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The LXCat project: Electron scattering cross sections and swarm parameters for low temperature plasma modeling

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ABSTRACT

LXCat is a dynamic, open-access, website for collecting, displaying, and downloading ELECtron SCATtering cross sections and swarm parameters (mobility, diffusion coefficient, reaction rates, etc.) required for modeling low temperature, non-equilibrium plasmas. Contributors set up individual databases, and the available databases, indicated by the contributor's chosen title, include mainly complete sets of electron-neutral scattering cross sections, although the option for introducing partial sets of cross sections exists. A database for measured swarm parameters is also part of LXCat, and this is a growing activity. On-line tools include options for browsing, plotting, and downloading cross section data. The electron energy distribution functions (edfs) in low temperature plasmas are in general non-Maxwellian, and LXCat provides an option for execution of an on-line Boltzmann equation solver to calculate the edf in homogeneous electric fields. Thus, the user can obtain electron transport and rate coefficients (averages over the edfs) in pure gases or gas mixtures over a range of values of the reduced electric fields strength, E/N, the ratio of the electric field strength to the neutral density, using cross sections from the available databases. New contributors are welcome and anyone wishing to create a database and upload data can request a username and password. LXCat is part of a larger, community-wide effort aimed at collecting, evaluating, and sharing data relevant to modeling low temperature plasmas. To illustrate the utility of LXCat in this context, we compare electron swarm parameters in argon calculated using the different compilations of cross sections presently available on LXCat. These compilations include quite different groupings of excited states, yet lead to swarm parameters in good agreement. LXCat is available at http://www.lxcat.laplace.univ-tlse.fr.

1. Introduction

The modeling of low temperature, non-equilibrium plasmas (LTPs) is centered on the description of electron transport since the energy gained by electrons in the sustaining electromagnetic fields is deposited in these plasmas mainly through electron-neutral collisions. The transport of electrons (and ions) and the coupling of the charged particle transport to electromagnetic fields can be described using different levels of models ranging from macroscopic "fluid models" [1], to "hybrid models" (see [2] for an overview of hybrid models), or to detailed kinetic models such as "particle in cell/Monte Carlo collision" (PIC–MCC) simulations [3]. Data needs for modeling depend on the level of description, but in all cases the needs are extensive. For PIC–MCC simulations, electron-neutral scattering cross sections are required input; the information required for fluid models includes electron transport and rate coefficients; and hybrid models use a combination of both kinds of data. Electron transport and rate coefficients are either measured or are calculated by averaging over the electron energy distribution function (edf), which is generally non-Maxwellian and is itself determined by solving the Boltzmann equation using cross section data as input.

There is a growing awareness in the LTP community that some means of collecting, evaluating and sharing data relevant to modeling cold plasmas is necessary [4]. Most modeling groups have their own collections of data and while people are generally willing

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to share, there has been no convenient way to exchange data except on an informal basis. Often the data concerning the electrons are in the form of compilations of electron-neutral scattering cross sections (up to nominally 1 keV) or tables of swarm parameters (transport coefficient-mobility, diffusion coefficient, reaction rates, etc.) as a function of E/N, the reduced electric field, the ratio of the electric field strength to the neutral density. LXCat (pronounced "elec scat" for ELECtron SCATtering) is a dynamic, open-access, website for collecting, displaying, and downloading the electron-neutral scattering cross sections and swarm parameters required for modeling low temperature plasmas. This website is intended to provide storage and access to data related to the electron component of low temperature plasmas as well as on-line tools to facilitate intercomparisons. Anyone willing to contribute data can request an account and instructions for setting up a database on LXCat. The contents and maintenance of the individual databases are the responsibility of the contributors. The LXCat site offers automatic daily back-up and usage statistics, and archived data is available upon request. For the users, the LXCat website provides options for browsing through databases, plotting, and downloading selected items from the databases. Also available on the LXCat site is an option for the on-line calculation of electron swarm parameters – electron transport and rate coefficients – in pure gases or in gas mixtures where cross section data for the component species are available in the LXCat databases. The swarm parameter calculation is based on BOLSIG+, an electron Boltzmann equation solver in the two-term approximation [5] and available as freeware [6]. A Monte Carlo simulation tool for LXCat is under development. A small, but growing, database of measured swarm parameters is expected to provide valuable points for comparison.

To be appropriate for use in Boltzmann or Monte Carlo calculations of the edf, the cross section data for a given target species must be complete. "Complete" in this context means that the cross section set be detailed enough to yield an accurate steady-state energy distribution for electrons subjected to the combined influences of a uniform electric field and collisions with a uniform density of neutral, ground-state target species. "Accurate" is difficult to quantify, but we generally demand that the cross section set, when used in a Boltzmann solver, yield swarm parameters to within 10% in pure gases. The accuracy test is normally conducted by comparison with experiment where available or by sensitivity tests when experiment is not available. In contrast, an incomplete or "partial" set of cross sections includes information about only one or a subset of the important scattering processes for a given species. Obviously, in different contexts, there could be other criteria for defining a "complete" set of cross sections.

In the following, we describe the LXCat website and illustrate its utility by intercomparisons of electron swarm parameters in pure argon calculated using the different compilations of cross sections presently available on LXCat.

The LXCat website is based on a modern LAMP system (Linux, Apache, MySQL, PHP) with an automatic backup. LXCat was designed to be continuously upgradable and users are encouraged to check back regularly for information regarding new features on the site and updates in the data.

2. Description of the website

LXCat is structured into individual databases, provided by different contributors, and on-line tools for manipulating the data, as illustrated in the graphical abstract above. At this writing, LXCat contains eight individual cross section databases belonging to seven different contributors. One of the databases (Biagi v8.9) is being extended to include more species (the original Biagi database includes 49 target species and only 5 have so far been transcribed from the original FORTRAN code format to the LXCat table format). Table 1 summarizes the available cross section databases in LXCat at the present time. The target species in each database (with the total number of scattering processes) are listed in the second column of Table 1, and further information is provided in the third column. Data for certain target species are common to several of the databases because of previous collaborations and informal data exchanges. At present, complete or partial sets of electron-neutral scattering cross sections are available in at least one of the databases on LXCat for the following 42 target species in their ground state: Ar, C, C_2H_2, C_2H_4, C_2H_6, C_3H_8, CCl_2F_2, CCl_4, CF_4, CH, CH_2, CH_3, CH_4, CHF_3, CO, CO_2, Cl_2, F_2, H, H_2, H_2O, HCl, He, Hg, Kr, Mg, N, N_2, N_2O, NH_3, NO, Na, Ne, O, O_2, O_3, SF_6, SO_2, $Si(CH_3)_4$ or TMS, Si_2H_6, SiH_4, and Xe. Some cross sections are available for electron collisions with atoms and molecules in excited states as indicated in Table 1.

Information for obtaining an account can be found on the LXCat site, and instructions for entering data in the databases are provided with the account information. The contents and maintenance of the individual databases are the responsibilities of the contributors. The LXCat website is presently set up to accept electron-neutral scattering cross sections (partial or complete sets) in tabular form and swarm parameters as functions of E/N.

Three levels of comments are included in the LXCat cross section databases – (a) comments the database as a whole, (b) comments for each target species and (c) comments for each individual process. The contributors (optionally) provide these comments. For the database as a whole, comments nominally include the names of the contributors with contact information, how the data should be used (two-term Boltzmann, Monte Carlo, etc.), and the suggested way to reference the data. For the individual target species, the comments contain, for example, references to publications or websites where the compilations have appeared. Finally, for each scattering process, the comments identify the states involved with references to original data sources as available. All three levels of comments appear in the text of downloaded data files because keeping proper references with the data is obviously very important. LXCat automatically introduces additional comments. The most recent change date for each cross section is automatically updated if contributors change/delete/upgrade the data. Databases are flagged with the status "maintenance" if anyone is logged onto the database account or if the data have been changed in the past hour. Note that contributors can manually set the status flag to "maintenance" or to "private". The latter flag is intended to be used while a database is under construction or if the owner wants to take it offline for any reason. The entire website is backed up on a daily basis, and archived versions are available by request.

3. How to use LXCat

Upon first entering LXCat, users can select from a variety of options in the top horizontal tool bar. The options include "how to use", "databases" for browsing through the databases with lists of species and first two levels of comments, "cross sections" for on-line plotting or downloading of selected data, "swarm parameters" to access experimental data or to effect an on-line Boltzmann calculation, and "notes" for more detail on certain related subjects. A Google group has been set up to encourage discussion among users.

Selecting the option "cross sections" and then "plot", for example, brings up the list of databases on the left. When the user selects one or more (or all) databases and clicks on "update list", the list of species for which data are available in the selected databases appears on the right. By selecting one or more species (and subsequently clicking on "update list"), the user is shown all the

Table 1
List of public databases available on LXCat at the time of writing. Other databases are under construction and include experimental electron transport data.

Database name	Target species (number of scattering processes included)	Comments
Biagi-v7.1	Extracted from Magboltz v7.1 Ar (5), He (4), Kr (6), Ne (11), Xe (6)	Extensive data compilations by S.F. Biagi, coded into his FORTRAN Monte Carlo code Magboltz [7]
Biagi-v8.9	More detailed cross sections for rare gases, extracted from Magboltz v8.9 Ar (46), He (51), Kr (6), Ne (47), Xe (52)	Compilations include cross sections for other species (49 total species), many of interest for radiation detectors. Tested using a Monte Carlo simulation, but in many cases a two-term Boltzmann solver yields swarm parameters with acceptable precision. The transcription of cross sections to LXCat for other target species is in progress
Bordage	CF_4 (7), CHF_3 (8), $Si(CH_3)_4$ (6)	Cross sections tested using a multiterm solution of the Boltzmann equation in the hydrodynamic approximation [8–11]
Drake	Detailed partial set of cross sections for excitation from the ground state to the first 4 excited states of argon. Ar(4)	From theoretical calculations using the Breit-Pauli B-spline R-matrix (BSR) method of Zatsarinny and Bartschat [12]. The observed near-threshold resonance structure [13] is well reproduced in these calculations
Hayashi	Ar (27), C_2H_2 (8), C_2H_4 (7), C_2H_6 (7), CCl_2F_2 (6), CCl4 (8), CF_4 (7), CH_4 (6), CO_2 (10), H_2O (8), HCl (6), N_2O (9), NH_3 (8), NO (10), Si_2H_6 (7), SiH_4 (7), SO_2 (6)	Compiled by M. Hayashi and tested using a Monte Carlo code. The argon data are from [14] and the other data were scanned and digitized from published curves [15,16]. For detailed references for individual species, see the LXCat site Note that a version of Hayashi's argon data, circulated informally for several years, contained an error in the elastic momentum transfer. This has been corrected on LXCat
Morgan	Ar (4), C (4), C_2H_2 (8),CF_4 (7), CH (3), CH_2 (3), CH_3 (3), CH_4 (11), Cl_2 (7), CO (18), CO_2 (13), F_2 (11), H (4), H_2(17), H_2O (10), HCl (8), He (4), Kr (4), N_2 (25), Ne (4), NH_3 (8), NO (10), O_2 (18), SF_6 (9), SiH_4 (7), Xe (4) Partial sets of cross sections for the following excited species and radicals: $H_2(p)$ (2), $H_2(s)$ (2), N (2), $N_2(a)$ (4), O (5), O_2 ($a^1\Delta$) (4), O_2 ($b^1\Sigma$) (4), O_3 (4), O^- (2)	An extensive collection of cross sections assembled over the course of 30 years by Morgan [17] and tested using the two-term Boltzmann solver, ELENDIF [18]. Some cross sections sets are described in Refs. [19–21] Morgan uses an analytical form to approximate the effect of a large number of rotational levels in the Boltzmann equation by a continuous function of the electron energy discussed by Frost and Phelps [22]. Note that this contribution to the rotational excitation has not yet been included in the data tables in the Morgan database on LXCat. This contribution is especially important for dipole molecules at low electron energy Some species are identical to those in the Hayashi database
Phelps	Ar (3), CO (18), CO_2 (13), H_2 (17), H_2O (5), He (3), Mg (4), N_2 (26), Na (7), Ne (8), NO (10), O_2 (17), SF_6 (9), Xe (3)	A compilation of atomic and molecular data assembled and evaluated by A.V. Phelps and collaborators. Tested using two-term Boltzmann analyses For detailed notes and references, the website [23]
SIGLO	Ar (3), CF_4 (7), Cl_2 (7), CO_2 (13), F_2 (11), H_2 (16), HCl (8), He (3), Hg (6), Kr (7), N_2 (25), Ne (8), O_2 (17), SF_6 (9), SiH_4 (7), Xe (8) Cross sections for ionization of metastables Ne(3p2) and Xe(1s5)	Assembled over many years and recently updated by the GREPHE team at LAPLACE in Toulouse. Distributed in various versions with the freeware two-term Boltzmann solvers, BOLSIG and BOLSIG+ [6] Some species are identical to those in the Phelps or Morgan databases

individual scattering processes for the selected databases/species combinations, and plots can be generated for selected subsets of the data in the lists. The plotting and downloading tools are useful for making comparisons (and have helped us identify mechanical errors that have crept into the various data compilations over the years). Cross section data can be selected and downloaded in a simple tabular format with a file header containing all descriptive comments and reference information provided by the contributors as described above. Users are requested to reference the database and the original references, where provided, in all publications making use of these data.

An especially useful feature in LXCat is the on-line version of BOLSIG+. BOLSIG+ [5] solves for the electron energy distribution function in the classical two-term approximation whereby the angular dependence of the edf in velocity space is assumed to be well-described by the sum of an isotropic and a cosine (with respect to the direction of the electron acceleration in the electric field direction) component. Swarm parameters and other useful quantities are calculated in BOLSIG+ by averaging different quantities over the edf. A good comparison of calculated and measured swarm parameters provides validation that the input cross section set is complete.

Selecting the option "swarm parameters" offers the possibility of browsing through the experimental database or calculating swarm parameters using BOLSIG+. Selecting "calculate" brings up again the list of databases on the left and species on the right, and selecting one or more species from the list calls up a dialog window for the on-line execution of BOLSIG+. The user then selects the range of values of E/N for the calculation and the components of the gas mixture and their relative concentration. The calculation is rapid and results appear in graphical format, and these swarm parameters can be downloaded in a convenient table form, with a text header giving the data used in the calculation. BOLSIG+ can optionally be used to calculate rate coefficient in an equilibrium (Maxwellian) plasmas.

Plasma modelers are confronted with the question of equivalence between swarm parameters and the coefficients needed for fluid models which seek to describe physical situations where there are density gradients, electric field gradients, physical boundaries, and other complications. Further questions arise concerning the exact definition of swarm parameters in different experimental configurations where electron number changing collisions (e.g. attachment and ionization) are present. While the latter questions have been discussed at length (see, for example, Ref. [24]) and are fairly well understood at this point, questions of equivalence of swarm parameters with coefficients used in fluid models merits further discussion. Concerning swarm parameters in different experimental situations, BOLSIG+ distinguishes between the calculations of swarm parameters in Pulsed Townsend (PT, exponential growth in time) configurations and Steady-State Townsend (SST, exponential growth in space) configurations. That is, when electron number changing processes (attachment and ionization) are present, BOLSIG+ assumes that only the magnitude, and not the shape, of the edf changes in time or in space, and the Boltzmann equation is rewritten to solve for the normalized distribution function. Where it is not possible to assume simply PT or

SST to describe the growth of the electron density, the corresponding Boltzmann equation is difficult to solve directly, and a Monte Carlo approach is usually preferred. The on-line version of BOLSIG+ assumes a Pulsed Townsend configuration; the freeware version of BOLSIG+ offers the option of a Steady-State Townsend configuration. The upcoming Monte Carlo option will have more flexibility.

4. Comparisons of calculated swarm parameters in argon

Many different compilations of cross sections in rare gases have been used over the years for the calculations of swarm parameters as discussed in the review paper of Petrović et al. [25]. See Refs. [26–32] for compilations of cross sections in argon other than those available in LXCat. Different criteria have been used to assess the validity of the compilations, the most appropriate for plasma modelers being the requirement that the cross sections, when used in a Boltzmann or Monte Carlo simulation, yield swarm parameters in good agreement with experimentally measured values. The data sets for argon in LXCat have all been used to obtain swarm parameters that generally compare well with experiment over a more or less limited range of values of E/N. Unfortunately, these comparisons are not carefully documented. Our purpose in this section is to illustrate the utility of LXCat by showing intercomparisons of swarm parameters in argon calculated with BOLSIG+ using the data presently available on LXCat. We will present comparisons between available experimental results and calculated swarm parameters in rare gases in a subsequent publication.

The cross section information used in two-term Boltzmann calculations is limited to momentum transfer cross section, total cross sections for inelastic processes, and the total cross section for ionization. Monte Carlo simulations and multi-term Boltzmann calculations take into account more detail about the anisotropy in the scattering cross sections, although lack of such additional information is generally not a factor limiting the accuracy of the swarm calculations [33]. Some authors refer to an "effective" momentum transfer cross section, and this is understood to be the sum of the elastic momentum transfer cross section and the total cross sections for inelastic and ionizing collisions [34,35]. The effective momentum transfer cross section is a quantity that appears naturally in the two-term approximation. LXCat uses the key words "elastic" and "momentum" to refer to "elastic momentum transfer" and "effective momentum transfer" cross sections, respectively. A better choice of keywords would be "elastic" and "effective", and we intend to phase in this change.

There are five, independently-compiled, complete sets of cross sections for argon on LXCat. The elastic momentum transfer cross sections for these five sets of data generally agree for energies below 11.55 eV, the first inelastic threshold. The width of the Ramsauer minimum is the same for all sets but its depth differs somewhat from one set to another (maximum difference is about 20%). Further small differences (about 5%) appear in the 7–10 eV region, and these have a slight but measurable influence on the calculated reduced mobility, μN, the product of the electron mobility and the gas density, as will be seen below. The ionization cross sections in the different databases differ essentially only in the energy resolution in the data tables, and we have confirmed that this has no effect on the calculated swarm parameters. These ionization cross sections are due to Rapp and Englander-Golden [36]. We note that the on-line Boltzmann solver in LXCat makes the assumption that the two electrons exiting the ionization events share equally the available energy whereas the freeware version of BOLSIG+ has more options. See Yoshida et al. [37] for an analysis of the influence of this assumption.

While the momentum transfer and ionization cross sections are quite similar in all five compilations in argon, there are considerable differences in the level of description of the excitation. The Phelps data for argon are the simplest of those in LXCat, considering only one effective excitation level. In his original database [23], Phelps also gives cross sections for excitation to the 2p7 and 2p9 levels, yielding radiation at 810.4 and 811.5 nm, respectively, and used for plasma diagnostics. These data could be used to calculate rate coefficients from a given distribution function, but are not to be used in the Boltzmann calculation because they are already included in the effective excitation. The argon compilation in the SIGLO database on LXCat is taken from Phelps.

The argon data in the Morgan database include two effective excited states – one for metastable excitation and a second effective level to account for all the other excitation. The momentum transfer cross section data in Morgan's original compilation extends to only 75 eV [17]. For energies greater than the highest value in the data tables, BOLSIG+ assumes all cross sections decrease with energy, ε, like $\log(\varepsilon)/\varepsilon$, consistent with the high energy limit of the Bethe–Born approximation [38]. This extrapolation is good for allowed transitions and for ionization, but it is incorrect for forbidden transitions, mixed transitions and for elastic momentum transfer, which all fall off much faster with energy. The contribution of these latter is usually so small at high energy, though, that the extrapolation has no effect.

The cross section compilation for argon [14] in the Hayashi database contains 25 excited levels, with 4 1s levels, 9 2p levels (2p4 and 2p5, separated by only 0.01 eV, are grouped into one level), and 12 levels grouping the other excited states, based on closeness of the threshold energy and high energy behaviour.

There are two sets of cross sections in argon compiled by Biagi on the LXCat website. Both sets were transcribed from his Monte Carlo code Magboltz [7], a set from Magboltz version 7.1, and the more recently compiled set, transcribed from version 8.9 of Magboltz. The transcriptions extend to 1 keV whereas the original data go to much high energy (100 keV in version 7.1 and MeVs in version 8.9). The Biagi-v7.1 argon cross sections include 3 excited states, corresponding to s, p and d levels, and were derived particularly for the s-state grouping. In 2009 Biagi revised his argon cross section compilation (Biagi-v7.1) in light of the recent calculations of Zatsarinny and Bartschat [12] which are in excellent agreement with the subsequent measurements of Allan et al. [13]. The resulting Biagi-v8.9 database includes 44 separate excitation levels in argon, with detailed resonance structures in the near-threshold region for the lowest five transitions. Their main effect is not due to the peaks but the general level of the cross section between the narrow peaks. In the higher energy region between the resonance region and 100 eV, Biagi uses electron scattering results [39–42] and data on the cross section section shape from light yields measured by the Wisconsin group [43–46]. The $J = 1$ levels above the resonance region have been deduced using the BEf scaling formula of Kim [47,48] which fit well to measured excitation cross sections. The triplet levels above 100 eV are scaled by $(\text{energy})^{-3}$ or $(\text{energy})^{-2}$ for mixed transitions.

While BOLSIG+ assumes that the electron energy distribution function is smooth between the energy grid points used in the calculation, no such assumption is made about the cross sections. Rate coefficients for each process are calculated using values of the cross sections at each of the energy values given in the input cross section tables. Thus the sharp resonance structures in the near-resonance regions in the lowest excited levels in argon are included in the calculations.

In spite of the different descriptions of the inelastic scattering, the electron reduced mobility μN vs E/N calculated using these different cross section sets are in good agreement among themselves. Values of E/N are shown in units of Townsend (Td) with 1 Townsend being equal to 10^{-21} V m^2. The maximum difference between the different calculated values of μN is 8% at about 7 Td, as shown

in Fig. 1, the highest value being from the Phelps compilation and the lowest value being from that of Hayashi. The good agreement is not really surprising since the cross section compilations have all been "validated" by comparisons with swarm parameters. We note, however, that the small differences in the results in Fig. 1 are experimentally observable. The measured quantity is the drift velocity, product of the μN and E/N, and the electron drift velocity can be measured with a precision of better than a few percent over a wide range of E/N. However, in order to accentuate the differences in the results by displaying them on linear scale, the mobility is shown rather than drift velocity. The two different Biagi databases yield identical results to within the resolution of the figure for the mobility and agree to within 1% for the subsequent figures. We therefore show results only from the Biagi v8.9 database in Figs. 1–4.

We show in Fig. 2 the characteristic energy, D/μ, ratio of the diffusion coefficient to the mobility where the diffusion coefficient is calculated as described in Ref. [5] using the classical two-term approach which yields a scalar diffusion coefficient. The characteristic energy is a measurable quantity [22] with units of energy, and although equal to the mean electron energy only in the limit of a Maxwellian distribution function, it provides an estimate of the electron energy scale vs E/N. Again, the different cross section sets yield very similar values, although there is more spread here than for μN in Fig. 1. This is not unexpected because D/μ is very sensitive to the details of the energy loss processes which are differently described in the five compilations whereas μN is more directly related to the effective momentum transfer which is essentially the same in each of the compilations.

The comparisons of the calculated fractional energy deposited in elastic, inelastic and ionization processes vs E/N are shown in Fig. 3. At low E/N all electron collisional energy loss goes into heating the gas through elastic collisions, and as E/N increases the electron energy lost is deposited mainly in the inelastic channels. Note the correlation of the rapid onset in the energy loss in inelastic channels with the structure in the curves for μN and D/μ which is especially noticeable at about 7 Td. Energy deposition in ionization is first noticeable on this scale at about 40 Td and increases thereafter.

In Fig. 4, we show the ionization rate coefficients calculated using the five different sets of cross sections. Except for the Morgan rate coefficient for E/N less than 100 Td, there is reasonable, but not perfect, agreement among the different calculations.

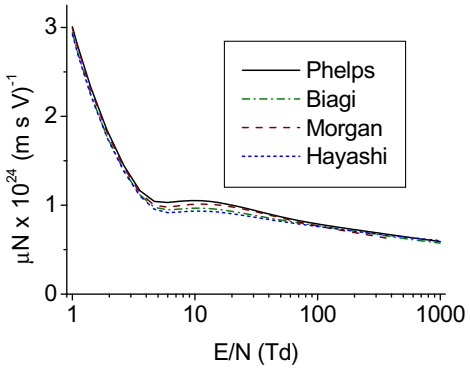

Fig. 1. Electron reduced mobility in argon vs E/N calculated using the different sets of cross sections as indicated.

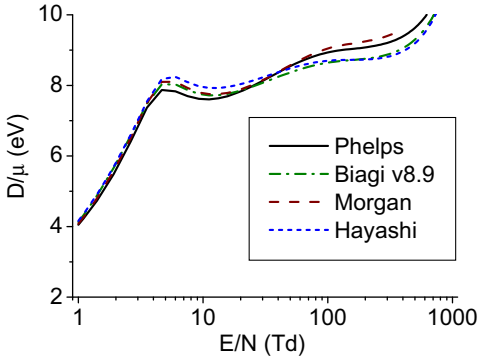

Fig. 2. Characteristic energy vs E/N in argon calculated using different sets of cross sections as indicated.

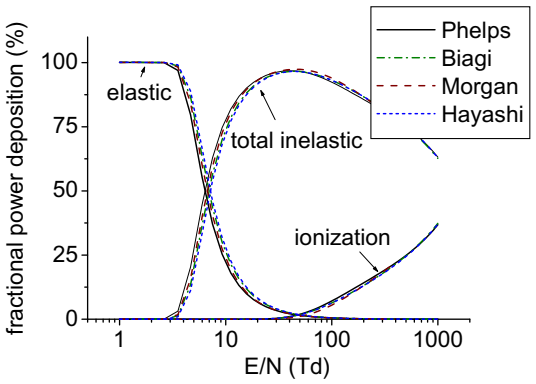

Fig. 3. Fractional power deposited into elastic, inelastic and ionization in argon vs E/N calculated using the different cross section sets as indicated.

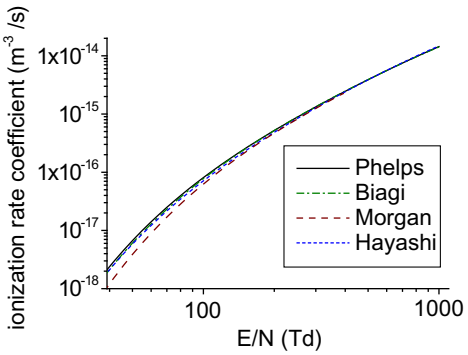

Fig. 4. Same as for Figs. 1 and 2, but showing the calculated ionization rate coefficients.

5. Conclusions

The question of the reliability of cross section sets made available by data sites such as LXCat encompasses issues of accuracy of transcription and presentation, timeliness, consistency, completeness, as well as of accuracy and energy resolution. For example, the comparison of electron–Ar cross sections made for this report led to the discovery that a more recent publication of Hayashi's momentum transfer cross section is significantly different than in the source previously used and is much more consistent with other compilations. The present comparisons of calculated swarm coefficients for electrons in Ar are an important step in evaluating the utility of the available sets. Future comparisons of Boltzmann calculations with experiments will serve as effective evaluations and recommendations to users. Results from some comparisons with experiment will be reported at the Plasma Data Exchange workshop to be held at the Gaseous Electronics Conferences in the USA in November 2011.

Additional data – both measured swarm data and cross section data - are being added to LXCat as new contributors are joining the project and as resources are available. The development of new tools is underway and users should check back from time to time for updates. A sister website for ion transport data is also on-line: www.icecat.laplace.univ-tlse.fr.

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References

[1] J.P. Boeuf, L.C. Pitchford, Phys. Rev. 3 (51) (1995) 1376.
[2] Z. Donko, P. Hartmann, K. Kutasi, Plasma Sources Sci. Technol. 15 (2006) 178.
[3] C.K. Birdsall, IEEE Trans. Plasma Sci. 19 (1991) 65.
[4] Low Temperature Plasma Science: Not only the Fourth State of Matter but All of Them, Report of the Department of Energy [USA], in: D.B. Graves, M.J. Kushner (Eds.), Office of Fusion Energy Sciences Workshop on Low temperature Plasmas, 2008.
[5] G.J.M. Hagelaar, L.C. Pitchford, Plasma Sci. Sources Technol. 14 (2005) 722.
[6] <http://www.bolsig.laplace.univ-tlse.fr>.
[7] <http://consult.cern.ch/writeup/magboltz/>.
[8] P. Ségur, M. Yousfi, M. Kadri, M.C. Bordage, Transp. Theory Stat. Phys. 15 (1986) 705.
[9] M.C. Bordage, P. Ségur, L.C. Christophorou, J.K. Olthoff, J. Appl. Phys. 86 (1999) 3558.
[10] M.C. Bordage, P. Ségur, A. Chouki, J. Appl. Phys. 780 (1996) 1325.
[11] M.C. Bordage, Plasma Sources Sci. Technol. 9 (2007) 756.
[12] O. Zatsarinny, K. Bartschat, J. Phys. B: At. Mol. Opt. Phys. 37 (2004) 4693.
[13] M. Allan, O. Zatsarinny, K. Bartschat, Phys. Rev. A74 (2006) 030701.
[14] Bibliography of electron and photon cross sections with atoms and molecules published in the 20th century – argon, National Institute for Fusion Research Research, Report NIFS-Data Series NIFS-DATA-72, Jan. 2003. In an appendix to this report Hayashi gives a set of recommended electron-Ar cross sections. The report cited is one of a NIFS series that reviews electron collisions with Xe, N_2, SF6, CO_2, etc.
[15] M. Hayashi, in: L.C. Pitchford, B.V. McKoy, A. Chutjian, S. Trajmar (Eds.), Swarm Studies and Inelastic Electron-Molecule Collisions, Springer-Verlag, New York, 1987, p. 167.
[16] M. Hayashi, in: M. Capitelli, J.N. Bardsley (Eds.), Nonequilibrium Processes in Partially Ionized Gases, Plenum Press, New York, 1990, p. 333.
[17] <http://www.kinema.com/data.htm>.
[18] W.L. Morgan, B.M. Penetrante, Comput. Phys. Commun. 58 (1990) 127.
[19] W.L. Morgan, Adv. At. Mol. Opt. Phys. 43 (2000) 79.
[20] W.L. Morgan, Plasma Chem. Plasma Proc. 12 (1992) 449.
[21] W.L. Morgan, Plasma Chem. Plasma Proc. 12 (1992) 477.
[22] L.S. Frost, A.V. Phelps, Phys. Rev. 127 (1962) 1621.
[23] <http://jilawww.colorado.edu/~avp/>.
[24] H. Tagashira, Y. Sakai, S. Sakamoto, J. Phys. D: Appl. Phys. 10 (1977) 1051.
[25] Z. Lj Petrović, S. Dujko, D. Marić, G. Malović, Ž. Nikitović, O. Šašić, J. Jovanović, V. Stojanović, M. Radmilović-Radenović, J. Phys. D: Appl. Phys. 42 (2009) 194002.
[26] C.M. Ferreira, J. Loureiro, J. Phys. D. Appl. Phys. 16 (1983) 1611.
[27] J. Bretagne, G. Callede, M. Legentil, V. Puech, J. Phys. D: Appl. Phys. 19 (1986) 761.
[28] K. Tachibana, Phys. Rev. A34 (1986) 1007.
[29] V. Puech, L. Torchin, J. Phys. D: Appl. Phys. 19 (1986) 2309.
[30] Á. Yanguas-Gil, J. Cotrino, L.L. Alves, J. Phys. D: Appl. Phys. 38 (2005) 1588.
[31] E. Gargioni, B. Grosswendt, Rev. Mod. Phys. 80 (2008) 451.
[32] <http://dpc.nifs.ac.jp/DB/IEEJ/>. This site states that the recommended data set for argon was compiled by The Institute of Electrical Engineers of Japan [in Japanese Report #853, Sep. 2001] and was chosen to reproduce measurements of transport data by using a two-term Boltzmann code.
[33] A.V. Phelps, L.C. Pitchford, Phys. Rev. A31 (1985) 2932.
[34] G.A. Baraff, S.J. Buchsbaum, Phys. Rev. 130 (1963) 1007.
[35] See Sec. II B L.C. Pitchford, A.V. Phelps, Phys. Rev. A25 (1982) 540.
[36] D. Rapp, P. Englander-Golden, J. Chem. Phys. 43 (1965) 1464.
[37] S. Yoshida, A.V. Phelps, L.C. Pitchford, Phys. Rev. A27 (1983) 2858.
[38] N.F. Mott, H.S.W. Massey, The Theory of Atomic Collisions, second ed., Oxford University Press, Oxford, 1952.
[39] D.M. Filipović, B.P. Marinković, V. Pejčev, L. Vušković, J. Phys. B: At. Mol. Opt. Phys. 33 (2000) 2081. and B33 (2000) 677.
[40] A.J. Chutjian, D.C. Cartwright, Phys. Rev. A23 (1981) 178.
[41] S. Proctor, M.A. Khakoo, J. Phys. B: At. Mol. Opt. Phys. 38 (2005) 929.
[42] M.A. Khakoo, P. Vandeventer, J.G. Childers, I. Kanik, C.J. Fontes, K. Bartschat, V. Zeman, D.H. Madison, S. Saxena, R. Srivastava, A .D. Stauffer, J . Phys. B: At. Mol. Opt. Phys. 37 (2004) 247.
[43] J.B. Boffard, B. Chiaro, T. Weber, C.C. Lin, At. Nucl. Data Tables 93 (2007) 831.
[44] J.E. Chilton, J.B. Boffard, R.S. Chappe, C.C. Lin, Phys. Rev. A57 (1998) 267.
[45] J.E. Chilton, C.C. Lin, Phys. Rev. A 60 (1999) 3712.
[46] T. Weber, J.B. Boffard, C.C. Lin, Phys. Rev. A68 (2003) 032719.
[47] Y.-K. Kim, Phys. Rev. A65 (2002) 022705.
[48] Y.-K. Kim, Phys. Rev. A64 (2001) 032713.